# SIMULATION OF PARTICLE SEGREGATION IN A BIDISPERSE SUSPENSION

**Raphaël PESCHE, Georges BOSSIS**
**and Alain MEUNIER**
*Laboratoire de Physique de la matière condensée*
*CNRS UMR 6622*
*Université de Nice-Sophia-Antipolis, 06108 Nice Cedex 2*
Tel: (33) 4 92 07 67 92 Fax: (33) 4 92 07 67 54

## 1. Introduction

It is now well known that a gradient in shear rate can induce particle migration in a concentrated suspension. Philips & al. (1992) have developed a constitutive equation for monodisperse suspensions based on the different shear induced diffusion mechanisms first described by Leighton and Acrivos (1987). This equation gives the equilibrium concentration profile from a balance between the primary flux, induced by shear rate gradients, and the secondary flux coming from concentration and viscosity gradients. Their model is in fair agreement with experimental results obtained by NMR imaging in a Couette geometry. In particular they recover, at steady state, a higher concentration in the lower shear rate region.

More recently, Chow & al. (1994) have also reported a migration towards higher shear rate region in a Couette flow but they did not observe such a phenomenon in parallel plate device contrary to the prediction of the model of Philips & al. The reason is that the constitutive equation of this model doesn't take into account the flux induced by the curvature of streamlines. Krishnan & al. (1996) have reported curvature contribution for bidisperse suspensions with one of the species being present only as tracer particles. A more general model for bidisperse suspensions was proposed recently by Bossis & al (1997) considering that the trajectory of the big particles were not perturbed by the small ones.

## 2. Basic models for suspensions in a Couette flow

We consider a suspension of spheres of radius a in a Newtonian fluid with viscosity $\eta$. We assume that the Reynolds number is sufficiently small for inertial forces to be negligible. On the other hand, we suppose that the spheres are large enough for Brownian motion to be negligible i.e. Peclet number (Pe $= 6\pi\eta a^3\gamma/ kT$) tends to infinity. The local shear rate $\gamma$ is due to the cylindrical Couette flow with the inner cylinder rotating with angular velocity $\Omega$.

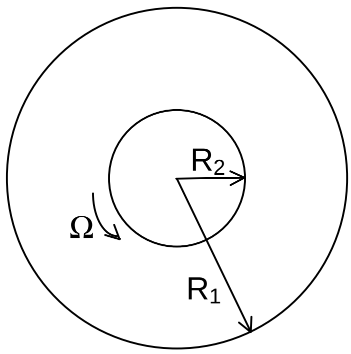



*Fig.1 Couette flow geometry*

### 2.1. Monodisperse suspension

We have to consider two different kinds of flux that cause particles migration. First, the effect of a spatially varying collision frequency in the gap between the cylinders gives rise to a flux $J_c$ :

$$J_c = -K_c a^2 (\Phi^2 \frac{d\gamma}{dr} + \Phi\gamma \frac{d\Phi}{dr}) \qquad (1)$$

$\gamma$ is the local shear rate. $K_c$ is a proportionality constant of order unity that is found from experimental data. We can see from (1) that even with no gradient in the particle volume fraction, migration will result because of the spatially varying shear rate. The minus sign indicates that the particles will migrate from high to low shear rate. The flux $J_c$ induces a non uniform particle volume fraction and therefore a spatially varying viscosity. This gives rise to another flux $J_\eta$ :

$$J_\eta = -K_\eta a^2 \gamma \frac{\Phi^2}{\eta} \frac{d\eta}{dy} \qquad (2)$$

$\eta$ is the local viscosity which is a function of the local volume fraction and $K_\eta$ is found from experimental data.
A conservation equation can be written in a Lagrangian frame as :

$$\frac{\partial \Phi}{\partial t} = -\nabla.(\Phi \mathbf{v} + \mathbf{J}) \quad (3)$$

Where $\mathbf{J} = \mathbf{J}\eta + \mathbf{J}_c$. With the condition of incompressibility and taking into account that the radial particles flux is zero on the boundaries, we must have at equilibrium :

$$\mathbf{J} = 0 \qquad (4)$$

The solution of eq. 4 with (1) and (2) gives the result of Philips & al.:

$$\frac{\Phi(r)}{\Phi_W} = \frac{r^2}{R_W^2} \left( \frac{1 - \Phi_W / 0.68}{1 - \Phi(r) / 0.68} \right)^{1.82(1 - K_\eta / K_C)} \qquad (5)$$

In this equation, $\Phi_W$ is the particles' concentration on one wall of the cylinders with radius $R_W$. We choose the empirical law for the relative viscosity (Krieger 1972):

$$\eta_r(\Phi) = \left( 1 - \frac{\Phi}{\Phi_{\max}} \right)^{-1.82} \qquad (6)$$

$\Phi_{max}$ being the volume fraction at which h tends to infinity, about 0.68 for hard spheres.
In equation (5) the quantity $K_c/K\eta$ is a parameter. It was found to be equal to 0.66 by Philips & al. Noting that 1.82 $(1-K_\eta/K_c) = -1$ allows to find the analytical solution of (5).

In contrast with the previous theory, migration has not been observed in a parallel plate device. In fact, we have to take into account the flux $\mathbf{J}_r$ due to the curvature of the streamlines (Krishnan & al., 1996) :

$$J_r = K_r \gamma a^2 \frac{\Phi^2}{r} \qquad (7)$$

In a parallel plate device, the particle volume fraction is initially constant (and therefore the viscosity), so $J_\eta = 0$ ( cf eq. (2) ) and the total initial flux is :

$$J = J_c + J_r = A(r)\,(K_r - K_c) \qquad (8)$$

As no migration has been observed experimentally (J=0), we shall take $K_r=K_c$.
Finally, imposing that the total flux (Eqs (1), (2), (7)) is zero, we obtain an equation for $\Phi$ including the participation of all the fluxes :

$$\frac{\Phi(r)}{\Phi_W} = \frac{r^3}{R_W^3}\left(\frac{1-\Phi_W/0.68}{1-\Phi(r)/0.68}\right)^{1.82(1-K_\eta/K_C)} \qquad (9)$$

*2.2 Bidisperse suspension*

In a further work we shall describe in more details the extension of Philips & al. theory for bidisperse suspensions with the addition of streamlines curvature flux. The only hypothesis is that the big particles are not perturbed by the small ones. We then rewrite the fluxes associated with the different kinds of collision and end up with two coupled equations for the volume fractions of big and small particles. In the next section of this work, we shall compare the predictions of the bidisperse model with a first numerical result we have obtained for a given ratio of sizes : $a_1/a_2=0.2$.

## 3. Numerical results

*3.1. Monodisperse system*

A Stokesian dynamic numerical method is used to simulate the whole system (Durlofsky & al., 1987). This method takes into account multi-body hydrodynamic interactions and the effects of lubrication layers between nearly touching particles. In order to save computing time we have simulated a monolayer of particles and therefore we only consider the two dimensional motion of the particles. The translational and rotational velocities of the spheres can be related to the hydrodynamic forces and torques ($\mathbf{F}_H$) exerted on the suspended spheres through the relations :

$$\mathbf{F}_H=\mathbf{R}(\mathbf{U}^\infty-\mathbf{U}) \qquad (10)$$

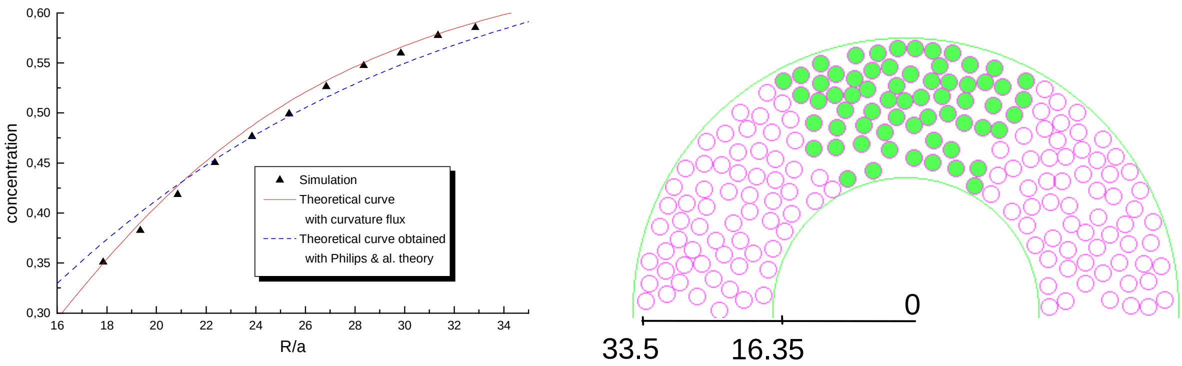
$\mathbf{U}$ contains the translational and rotational velocities of the N suspended particles ; $\mathbf{U}^\infty$ contains the translational and rotational components of the bulk velocity that would exist at the centre of the particles in the absence of the particles.
The coefficients in the matrix **R** can be found in Jeffrey & al. (1984, 1992). Because of the presence of the cylinders walls, we have to introduce the particle-wall interactions as in Bossis & al. (1991).

In addition to hydrodynamic interactions we have to take into account a repulsive potential which can be related to the rugosity or ionic repulsion between particles. An

important point is that this potential introduces an asymmetrical trajectory between two spheres.
We choose a pairwise repulsive DLVO-type colloidal force of the form (Brady and Bossis, 1988):

$$F^{ab} = \tau F_0 \frac{e^{-\tau\varepsilon}}{1-e^{-\tau\varepsilon}} \qquad (11)$$

$F^{ab}$ is the force on particle a due to particle b, ε is the separation between the particle surfaces, τ is the Debye length which gives the range of the repulsive force. In this work, we have taken $1/\tau = 2.2\ 10^{-3}$ radius.
The amplitude $F_0$ is chosen in order to obtain hydrodynamic forces between particles a and b equal to $F^{ab}$ when the surface separation is 0.01 radius.




(a) (b)

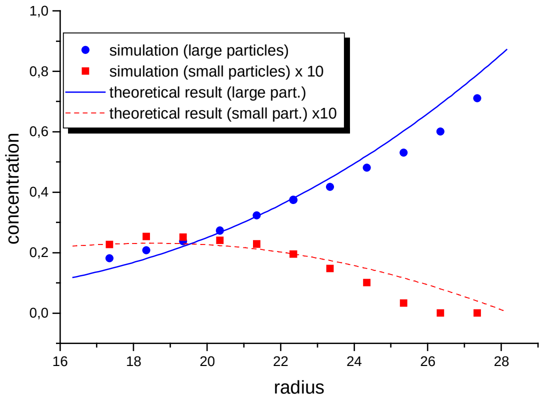
*Fig.2: Results obtained for a monodisperse suspension with mean volume fraction $\overline{\Phi}$ = 0.5. (a) concentration profile compared with theoretical prediction ; (b) picture of half Couette system. The full spheres are those taken into account in the calculations. The others are obtained with angular periodicity. Units are in particle's radius.*

In Fig. 2 (a), our numerical simulation is compared with an analytic solution obtained by solving equation (9) taking $K_c/K_\eta$ =0.66 as proposed by Philips. The quantity $\Phi_w$ is obtained from the condition that the integral of the volume fraction gives the average volume fraction. The dotted line is the prediction of Eq. (5) whereas the solid line is the prediction of Eq. (9). It appears that the inclusion of the radial flux markedly improve the model.

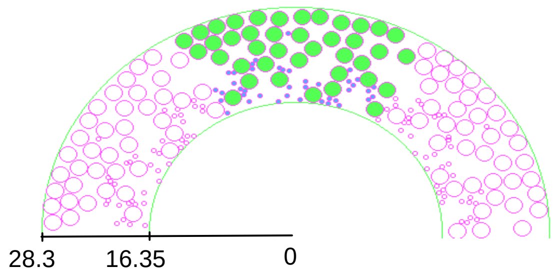
### *3.2. Bidisperse system*

We apply the same numerical method with two different sizes of spheres of radius ratio $a_1/a_2$=0.2. The functions that we need to build have been studied by Jeffrey for unequal rigid spheres.

We observe a strong segregation in sizes with larger particles migrating towards lower shear rate region (i.e. the outer cylinder). The concentration profiles are plotted (solid dots for large particles and solid squares for small particles in fig. 3a).




(a)




(b)

*Fig. 3 : Results obtained for a bidisperse suspension with mean volume fraction $\overline{\Phi} = 0.45$ (large spheres) and 0.02 (small spheres). The radius ratio $a_1/a_2$ is 0.2. (a) concentration profile compared with theoretical prediction ; (b) picture of half Couette system. Units are in large particle's radius (i.e. $a_2$).*

The theoretical curves obtained from our model are respectively the solid line and the dotted line for the big and the small particles. The agreement is fair especially taking into account that the only parameter of the bidisperse model is the same as for the monodisperse one ($K_c/K_\eta$ =0.66).

## 4. Phase separation under simple shear rate

We also performed simulation of a 2 dimensional bidisperse system undergoing simple shear flow in order to determine the importance of hydrodynamic interactions.

4.1 Without hydrodynamic interactions between particles

Suspended particles interact each other with a Debye-Huckel (see Russel & al., 1989) repulsive force ($F^{rep}$). Each particles undergoes a Stokes drag force $F^{\eta}$ as if it were alone in the fluid. At each time step, we have :

$$F^{rep} + F^{\eta} = 0 \qquad \text{(neutrally buoyant particles)}$$

The velocity of the particles is given by :

$$\mathbf{v} = \frac{\mathbf{F}^{rep}}{6\pi a \eta} + \gamma y \mathbf{e_1}$$

With a velocity in the x-direction due to the shear given by $\gamma y$ ; a is the radius of a particle and $\eta$ the viscosity of the fluid.

Figure 4 shows that the system becomes stripe structured. Santra & al. (1996) have obtained such a phase separation taking into account inertia of particles.

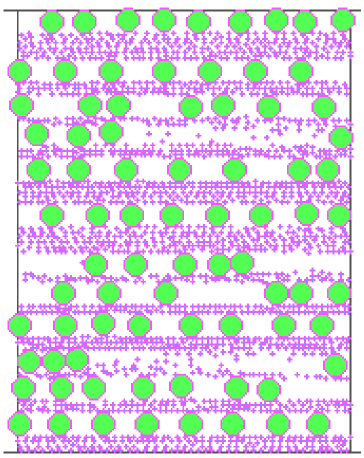
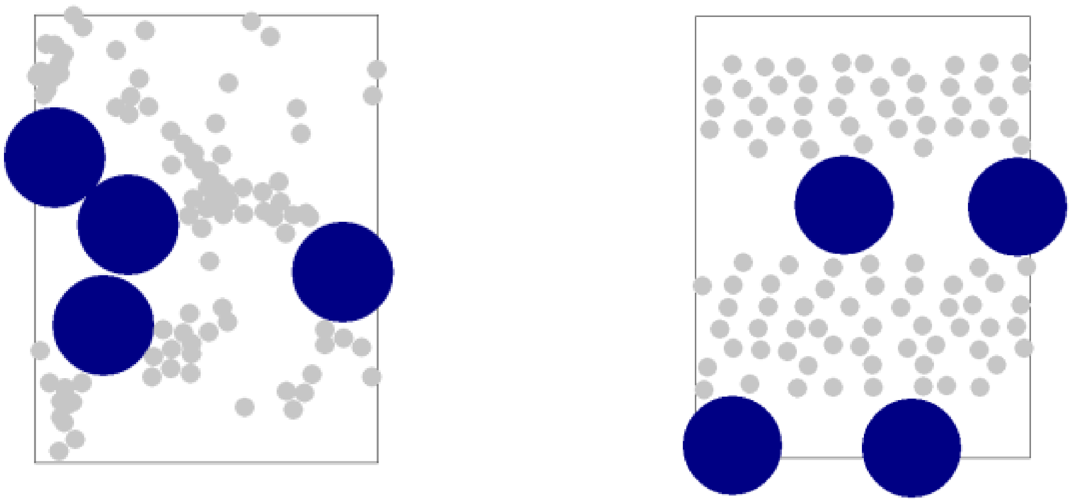


*Fig. 4 : 2000 particles, $\phi_B$=0.21, $\phi_S$=0.20 (surface concentration of big and small* particles) at dimensionless time $\gamma t$ = 400.

4.2 Effect of hydrodynamic interactions between particles

We performed numerical simulation of the same system including a Stokesian Dynamic method (Durlofsky & al., 1987). Because of the computational time increasing, we used a small number of particles. Figure 5 allows to compare the effect of hydrodynamic interactions - that make little clusters of aggregating particles and prevents the stripes formation - with the case of a single repulsive force.



(a) (b)

*fig. 5 : Results obtained for a bidisperse suspension with mean volume fraction* $\overline{\Phi}$ *= 0.42. (a) agregations caused by lubrication forces. (b) stripes when lubrication forces are replaced by short ranged repulsive forces.*

## Conclusion

We have developed a numerical simulation including many body hydrodynamic interactions which allows to reproduce particle's migration in a monodisperse or a bidisperse suspension placed in a two dimensional Couette flow. The concentration profiles obtained by numerical simulation have been compared to the predictions of models based on the ideas of Leighton and Acrivos. For monodisperse suspensions it appears that taking into account the flux due to the curvature of streamlines well improve the agreement of the model with the numerical simulation. In the bidisperse case for a ratio of sizes $a_1/a_2=0.2$, we observe a strong segregation with the large particles going towards the lower shear rate gradients. Our model for bidisperse suspensions fairly well predicts this behaviour without the addition of others parameters. The comparison between numerical simulations and the bidisperse model will be worked out for different size ratios and volume fractions.

Concerning the phase separation in bidisperse 2D suspension under simple shear rate, we perform now a theoretical interpretation including diffusion coefficients in order to predict the appearance of stripes depending on the radius ratio and concentration of the spheres.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